

1,2,4,6,8,8-Hexachloro-1,1,2,3,3,4,5,5,6,7,7,8-dodeca-

octane

Inchi:	InChI=1S/C8Cl6F12/c9-1(15,5(20,21)3(11,17)8(14,25)26)4(18,19)2(10,16)6(22,23)7(12,13)
InchiKey:	NHRNQFMRKUFJPZ-UHFFFAOYSA-N
Formula:	C8Cl6F12
SMILES:	FC(F)(Cl)C(F)(Cl)C(F)(F)C(F)(Cl)C(F)(F)C(F)(Cl)C(F)(F)C(F)(Cl)Cl
Mol. weight [g/mol]:	536.78
CAS:	335-68-2

Physical Properties

Property code	Value	Unit	Source
gf	-2370.10	kJ/mol	Joback Method
hf	-2726.21	kJ/mol	Joback Method
hfus	19.31	kJ/mol	Joback Method
hvap	39.54	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	7.539		Crippen Method
mcvol	218.260	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
tb	572.42	K	Joback Method
tc	750.56	K	Joback Method
tf	385.88	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.62	J/molxK	572.42	Joback Method
cpg	533.16	J/molxK	602.11	Joback Method
cpg	540.48	J/molxK	631.80	Joback Method
cpg	546.70	J/molxK	661.49	Joback Method
cpg	551.93	J/molxK	691.18	Joback Method
cpg	556.31	J/molxK	720.87	Joback Method
cpg	559.95	J/molxK	750.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C335682&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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